DOCTORAL THESIS

Metallopolyyne polymers of plantinum (II) as new functional materials for photovoltaic and solar cell applications

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Metallopolyyne Polymers of Platinum(II) as New Functional Materials for Photovoltaic and Solar Cell Applications

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Abstract

The molecular design, synthesis, spectroscopic and photophysical characterization of a series of new platinum(ll)-containing complexes and polymers incorporating various functional chromophores are discussed. These metallopolyyne polymers of platinum(II) as new functional materials for photovoltaic and solar cell applications are also outlined.

Chapter 1 contains a brief overview on the background of platinum-containing polymers and complexes and their role in the fields of photovoltaic and polymer solar cells. It also presents an overall review of progress in organic photovoltaics cells (OPVs), including the device architecture and the parameters used to characterize the performance of photovoltaic devices.

Chapter 2 presents the design and the synthesis of a series of soluble conjugated metallopolymers, consisting of a fluorenone central unit symmetrically coupled to oligothiophene segments, which can be efficiently used as donor components in PCBM-based bulk-heterojunction solar cells. A full account of the preparation, characterization, photophysical and thermal properties of a new series of metallopolyyne polymers of platinum(II) and their model complexes are presented.

Finally, we describe their performances in photovoltaic cells with respect to the differences in chemical structures and molecular weights. Optimization of the devices yielded the cell power conversion efficiencies (PCEs) up to 4.8%.

In Chapter 3, we report the design and synthesis of a series of conjugated donor-acceptor metallated conjugated polymers, consisting of thiadiazole, selenadiazole and bithiazole-based central unit symmetrically coupled to oligothiophene segments, which can be efficiently used as donor components in methanofullerene-based bulk-heterojunction solar cells. The solubility and the film-forming ability of the newly synthesized molecules are improved by the presence of hexyl chains in the oligothiophene units. The effect of thienyl chain length on improving the polymer solar cell efficiency and their optical and charge transport properties is elucidated in detail. The power dependencies of the solar cell parameters (including the short-circuit current density, open-circuit voltage, fill-factor and PCE) were also examined. The solar cell behavior has been extensively investigated and the best efficiencies even without thermal annealing can reach up to 4.1%. The present work opens up an attractive avenue to developing conjugated metallopolymers with broad solar absorptions and tunable solar cell efficiency and supports the potential of metallated conjugated polymers for efficient power generation

Chapter 4 outlines the synthesis, structural, photophysical and electrochemical properties of a novel family of multifunctional platinum(II) donor-acceptor low-bandgap metallopolymers containing thienopyrazine-thiophene, cyclopentadithiophene-thiophene and 3,4-ethylenedioxythiophene-benzothiadiazole spacers. Optical spectroscopy and electrochemical studies suggest very narrow bandgap systems for all polymers. Metallated polymers with extremely low bandgaps are thus achievable to meet a greater flexibility in the solar cell design. Photovoltaic cells with spectral responses up to about 900 nm were fabricated and investigated in detail and the broad photocurrent spectral responsivity would make them suitable for efficient light harvesting and charge-carrier extraction in PSCs. Photovoltaic properties of the material were initially investigated, and a PCE of up to 0.63% was observed under illumination of AM1.5 from a solar simulator and this work represents the first demonstration of efficient near-infrared photocurrent spectral responses for metallopolyynes.

Chapter 5 and 6 present the concluding remarks and experimental details of the work described in Chapters 2–4.

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